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FINAL REPORT

on

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A SPACE-MARCHING ALGORITHM FOR THE PARABOLIZED NAVIER-STOKES EQUATIONS WITH CHEMISTRY - PHASE 3

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Unclas Z9/61 0084788 Installation 1.1
3/30/92

This version of gasp is setup to run identically in a number of different unix environments. (Our main development environments are Cray Y-MP, and SGI workstations however, compilation requires the use of different compilation flags All Makefiles make use of the "include" option to incorporate machine dependent parameters.

The file Makefile.def in the main gasp directories contains all machine specific parameters. i.e. optimization flags, and compiler names are contained in this file. Several default configurations may be found in the Makedef directory. in order to extract the default machine configuration file simply type make "machine type" for example make iris will copy the appropriate configuration file for ieee workstations make cray5 is suitable for cray operating systems with cf77 vs 5.x (NAS Crays) make cray4 is suitable for cray operating systems with cf77 vs 4.x (Langley Crays) make convex is suitable for convex operating systems

Note, the compilation flags are suitable for default optimization if debugging is desired modify the FFLAGS & CFLAGS variables from Makefile.def, it is not necessary to modify the Makefile in the source directory

Note: The makefiles in the source directories should not require modification for machine dependent parameters, only make modifications to Makefile.def to port to different hardware/software environments

COMPILATION:

in order to compile the gasp execution environment, first select the machine appropriate for you, and type from the main gasp directory 'make MACHINENAME'

edit the Makefile.def file and make appropriate modification to the compiliation flags.

then type

'make install'

(this will compile the gasp CFD flow solver, print the post-processor and dbasemgr, the utility used to build the chemistry and thermodynamics database, finally, the chemistry and thermodynamics database will be created.

all executables will be installed in the bin directory. everything is now ready to run your own problems or any of the test cases located in the samples subdirectory

```
input.bouns 1.1 3/30/92
```

boundary condition files if any of the boundaries, IO, Idim, JO, Jdim, KO, Kdim have type 0, then a pointwise boundary condition file must be specified. This file must contain a boundary condition flag for each face on the boundaries with bc type 0 note there are (jdim-1)*(kdim-1) faces on the IO, and Idim boundaries (kdim-1)*(idim-1) faces on the JO, and Jdim boundaries (idim-1)*(jdim-1) faces on the KO, and Kdim boundaries the logic for reading these flags is if (boundary condition for IO boundary = 0) then read(from bci file) ((i0 boun type(j,k),j=1,jdim-1),k=1,kdim-1) end if if (boundary condition for Idim boundary = 0) then read(from bci file) ((idim boun type(j,k), j=1, jdim-1), k=1, kdim-1) end if if (boundary condition for J0 boundary = 0) then read(from bci file) ((j0 boun type(k,i),k=1,kdim-1),i=1,idim-1) end if if (boundary condition for Jdim boundary = 0) then read(from bci file) ((jdim_boun_type(k,i),k=1,kdim-1),i=1,idim-1) end if if (boundary condition for KO boundary = 0) then read(from bci file) ((k0 boun type(i,j),i=1,idim-1),j=1,jdim-1) end if if (boundary condition for Kdim boundary = 0) then read(from bci file) ((kdim_boun_type(i,j),i=1,idim-1),j=1,jdim-1) end if NOTE: the reading of the j0 and jdim boundaries is different from that in gasp1.x if any of the boundaries face has bc type 2, then the q for that face must be read in from the boundary condition q file

Note, either the global boundary condition flags may

to type 2.

be set to type 2, or the pointwise boundary conditions may be set

```
the format for the q file is one set of q's per line
the q's must be specified in primitive variables in dimensional
quantities appropriate for the iunits flag specified in the main
input deck
first are all nspec densities, then u, v, and w, and finally pressure.
NOTE: the temperature is not required as with gasp 1.x
the following provides a flow chart of the input of the boundary q's
for k = 1 to kdim-1
   for j = 1 to jdim-1
     if ( ( boundary condition for IO boundary = 2 )
         ( boundary condition for IO boundary = 0 )
           and pointwise boundary condition for point j,k=2) ) then
         read(from bc q file) (qbci0(j,k,ne),ne = 1,neqn)
      end if
   end for j
end for k
for k = 1 to kdim-1
   for j = 1 to jdim-1
     if ( ( boundary condition for Idim boundary = 2 )
         (boundary condition for Idim boundary = 0)
           and pointwise boundary condition for point j,k=2) then
         read(from bc q file) (qbcidim(j,k,ne),ne = 1,neqn)
      end if
   end for i
end for k
for i = 1 to idim-1
   for k = 1 to kdim-1
     if ( ( boundary condition for J0 boundary = 2 )
         (boundary condition for J0 boundary = 0)
           and pointwise boundary condition for point k,i = 2) ) then
         read(from bc q file) (qbcj0(k,i,ne),ne = 1,neqn)
      end if
   end for k
end for i
for i = 1 to idim-1
   for k = 1 to kdim-1
     if ( ( boundary condition for Jdim boundary = 2 )
         ( boundary condition for Jdim boundary = 0 )
           and pointwise boundary condition for point k,i = 2) ) then
         read(from bc q file) (qbcjdim(k,i,ne),ne = 1,neqn)
```

```
end if
   end for k
end for i
for j = 1 to jdim-1
  for i = 1 to idim-1
     if ( ( boundary condition for KO boundary = 2 )
         ( boundary condition for KO boundary = 0 )
           and pointwise boundary condition for point i, j = 2) ) then
         read(from bc q file) (qbck0(i,j,ne),ne = 1,neqn)
      end if
   end for i
end for j
for j = 1 to jdim-1
   for i = 1 to idim-1
     if ( ( boundary condition for Kdim boundary = 2 )
         ( boundary condition for Kdim boundary = 0 )
           and pointwise boundary condition for point i, j = 2) then
         read(from bc q file) (qbckdim(i,j,ne),ne = 1,neqn)
      end if
   end for i
end for j
NOTE: the reading of the j0 and jdim boundaries is different from
      that in gasp1.x
```

DBASEMGR

Introduction:

DBASEMGR is a management program for the GASP databases. This program takes ordinary text files (called init files) and converts them into direct access files for use by GASP. This document describes how to install, run, and configure the database manager

Quick Installation & Execution:

When you first make gasp, the database manager will also be compiled and run for the first time. During this initial run it will create, summarize, and perform extended error analysis on the databases. You will see messages from the program during each phase of the execution. Seven files are created during the initial execution, the three databases, three summary files, and a log file. Each of these files are explained later in this documentation.

Configuration:

DBASEMGR has several options which tell the program what to do. The options are specified in the file dbasemgr.cnf. This file must reside in the current working directory (the directory where the init files reside). If this file does not exist then the program will create a default configuration file and use the default values during execution. It is recommended that you allow DBASEMGR to create a default configuration file and then edit the file to change the way the program operates.

The configuration file has the following format:

- Line 1: Title (ignored)
- Line 2: Title (ignored)
- Line 3: Names of the reaction, species, and models init (ascii) files.
- Line 4: Title (ignored)
- Line 5: Names of the reaction, species, and models database files.
- Line 6: Title (ignored)
- Line 7: Names of the reaction, species, and models summary files.
- Line 8: Title (ignored)
- Line 9: Names of the reaction, species, and models addition files.
- Line 10: Title (ignored)
- Line 11: Names of the reaction, species, and models extraction files.
- Line 12: Title (ignored)
- Line 13: Flag for creating the Liu files, the names of the Liu ascii file and binary file respectively.
- Line 14: Title (ignored)
- Line 15: Name of the log file for errors.
- Line 16: Title (ignored)
- Line 17: Overwrite variable.
- Line 17: Title (ignored)
- Line 18: Mode which tells the program what to do next.

 There can be up to 10 modes, each on a separate line.

Files:

[ASCII Init Files]

The "init" files are the initialization files used by DBASEMGR to create the binary databases for GASP. The init files are broken down into three separate files, one for the reactions, one for the species, and one for the models.

The format of the REACTIONS INIT file is as follows:

```
Line 1: Title (record separator - ignored)
  Line 2: Title (ignored)
  Line 3: Reaction number and reaction in symbolic form
  Line 4: Title (ignored)
  Line 5: Rate calculation flag and reference
Line 6: Title (ignored)
Line 7: Forward rate coefficients
  Line 8: Title (ignored)
  Line 9: Equilibrium rate coefficients
  Line 10: Title (ignored)
  Line 11: Title (ignored)
  Line 12: Title (ignored)
  Line 13: Title (ignored)
  Line 14: Title (ignored)
  Line 15: Stoichiometric Coefficients (Left Hand Side)
  Line 16: Stoichiometric Coefficients (Right Hand Side)
The rate calculation flag is equivalent to icheq in GASP. The
following values are currently supported:
  icheq = 1 Arrhenius equilibrium rate
  icheq = 2 Park equilibrium rates
  icheq = 3 Equilibrium rate calculated from LeRC curve fits from
             Gibbs free energy.
All forward rates are calculated using Arrhenius form.
For icheq = 3, line 9 is treated as a dummy title.
The format of the SPECIES INIT file is as follows:
Line 1: Title (record separator - ignored)
Line 2: Title (ignored)
Line 3: Species number
Line 4: Title (ignored)
Line 5: Species symbol and molecular weight
Line 6: Title (ignored)
Line 7: Control flags (ibmu, ismu, isk, ilrc, ivib)
Line 8: Title (ignored)
Line 9: Title (ignored)
Line 10:
       : LeRC Coefficients (Lower Range)
Line 19:
Line 20: Title (ignored)
Line 21:
       : LeRC Coefficients (Upper Range)
Line 30:
Line 31: Title (ignored)
Line 32: Blottner coefficients for laminar viscosity
Line 33: Title (ignored)
Line 34: Sutherland coefficients for laminar viscosity
Line 35: Title (ignored)
Line 36: Sutherland coefficients for thermal conductivity
Line 37: Title (ignored)
Line 38: Number of vibrational temperatures
Line 39: Title (ignored)
Line 40: Vibrational Temperatures (All on single line)
The control flags specified on line 7 allow one or more of
the coefficients to be left out for a given species. For example,
if ibmu is set to zero then lines 31-32 should not be present.
The control flags have the following meaning:
    ibmu - read Blottner viscosity coefficients
   ismu - read Sutherland viscosity coefficients
   isk - read Sutherland thermal conductivity coefficients
```

ilrc - read Lewis Research coefficients (McBride coefficients) ivib - read vibrational temperatures

The format of the MODELS INIT file is as follows:

Line 1: Title (record separator - ignored)

Line 2: Title (ignored)

Line 3: Model number and model name

Line 4: Title (ignored)

Line 5: Number of species and reactions for the model

Line 6: Title

Line 7: List of species in model. Each species is specified by the number in the species init file. Each must be placed on a separate line.

Line 8: Title (ignored)

Line 9: List of reactions in model. Each reaction is specified by the number in the reactions init file. Each reaction must be placed on a separate line.

[Database Files]

These are the files that are read in and used by GASP to retrieve information about a given model, species, or reaction.

[Summary Files]

The summary files contain useful information about the different databases. There are three summary files, one for each database.

[Extraction Files]

The extraction files are the same as the init files except that these are created from the binary database files. These files can be used as the init files after a record has been added to one of the databases (See adding species for more details)

[Report Log]

This is where all errors are logged. If the program complains about a possible error during the analysis phase, it will tell you to look in this file for more details. At the end of the file is a list of the models with the valid thermodynamic, laminar viscosity, and laminar thermal conductivity models for each model.

Modes:

There are 10 different modes that are valid.

help Prints listing of all valid modes. If an invalid mode is chosen this

message will be printed.

create Create GASP databases

summary Print summaries of the databases

summarize Same as summary

extract Extracts the init files from the databases

Warning!

Adding species:

Adding species should always be handled by DBASEMGR. the other two databases are dependent on the species database these databases will have to be modified to reflect the addition of a species. When a species is added with DBASEMGR, the reactions and models database are modified to reflect the changes in the species database. After adding species it is recommended that new init files be created using the extract mode. The new init files can then be edited to add models and reactions.

input.main 1.1 3/30/92

Terminology used in GASP Input Decks:

Zone - a section of the computational domain that is described by an individual zonal input deck

Zonal Boundary - a physical boundary between two zones across which information is passed

Group - a group of zones that are run simultaneously because solution information is shared between the zones in that group during the iteration process of the group.

Sequence level - the level of coarsening for a group of zones

Block - A block is described as a given group on a given sequence level

Marching - space marching which performs an iteration on a single plane of a given group at a time

Global iteration - performs an iteration on all planes of a given group at a time

GASP has multiple input decks. It has a main controller input deck and also individual input decks for each zone in a given problem. Below is a brief description of the input decks.

Main input deck description

The main input deck is broken down into 5 main sections:

- 1) Main info describes the problem as a whole
 - a) reference quantities
 - b) file control parameters
 - c) number of zones, zonal boundaries, groups
- 2) Zone info describes zone dependent information
 - a) zone file names
 - b) surrounding zonal boundaries
- 3) Zonal Boundary info describes zonal boundary information
 - a) grid alignment for boundaries
 - b) variable mapping for boundaries
- 4) Group info describes group dependent information
 - a) starting & ending zones
 - b) marching vs global iteration
 - c) mesh sequencing levels
- 5) Block info describes solution process

- a) group & sequence level
- b) # of cycles & convergence criteria
- c) sweeping information

Each of these sections is divided in this file by a line that has the section name surrounded by #'s.

-----DUMMY LINE ------

******************* main info line 2 *****************

iunits - unit specification flag

= 0 English Units

= 1 SI Units

rhoref - reference density (slugs/ft^3 or kg/m^3)

vref - reference velocity in (ft/s or m/s)

tref - reference temperature in (degrees R or Degrees K)

lref - reference length (ft or m)

NOTE: These are only used for non-dimensionalization in GASP. They are not related to the freestream values. You may choose the reference quantities any way you want. If you set them all to 1., then the calculations are all performed with dimensional variables. You may choose to set them such that your non-dimensional freestream variables are order one.

NOTE: The grids you provide must be non-dimensional thus if your grid is in feet and iunits = 0 select lref = 1. however if you grid is in yards lref must be set to the foot equivalent of 1 yard or lref = 3.

irest - flag for restart

- = 0 no restart
- = 1 restart

memmode - memory mode

- = 0 low memory mode, use minimum memory at expense of i/o
- = 1 medium memory mode, middle of the road trade-off between low & high
- = 2 high memory mode, use enough memory to minimize i/o

filmode - format of grid and restart files

= 0 c - binary

= +- 2 - output group and zone information = +- 4 - output group, zone, sweep, and plane info
- + - 3 - output group zone and sweep, and plane info
- +- 3 - output group zone and sweep information - +- 4 - output group, zone, sweep, and plane info
= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info
- +- 3 - output group zone and sweep information - +- 4 - output group, zone, sweep, and plane info
- +- 3 - output group zone and sweep information - +- 4 - output group, zone, sweep, and plane info DUMMY LINE ***********************************
= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info ***********************************
= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info
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= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info
= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info
<pre>= +- 3 - output group zone and sweep information = +- 4 - output group, zone, sweep, and plane info</pre>
= 0 no residual information = +- 1 - output group residual information
positive numbers indicate all residual information to a single file negative numbers indicate residual information to individual files
= 1 fortran formatted binary, direct access resmode - level of restart files

zone # - zone #'s in increasing order

enclose file name in 'single quotes' filedir - storage direction for zonal grid & restart files = 1 - grid & restart stored (jdim, kdim, idim) = 2 - grid & restart stored (kdim, idim, jdim) = 3 - grid & restart stored (idim, jdim, kdim) gridfil - file name for zonal grid file enclose file name in 'single quotes' restfil - file name for zonal restart file enclose file name in 'single quotes' ------DUMMY LINE ------******************* zone info line 2 ****************** zone # - zone #'s in increasing order fillzb - flag for initializing a zone with a given zonal boundary = 0 do not initialize in this way = 1 initialzes with i0 zonal boundary = 2 initialzes with idim zonal boundary = 3 initialzes with j0 zonal boundary = 4 initialzes with jdim zonal boundary = 5 initialzes with k0 zonal boundary = 6 initialzes with kdim zonal boundary # surr. zones - # of zonal boundaries around a given zone zb1, zb2,...zbn - the corresponding numbers of the zonal boundaries (in list above) that surround a given zone. ******************* end of zone info ****************** ######################### ZONAL BOUNDARY INFO ################################# -----DUMMY LINE -------The next SET of lines repeats for each zonal boundary (NZBOUN times) ------ DUMMY LINE ----------- DUMMY LINE ------**************** zonal boundary line 1 *************** zone# - zone # on one side of zonal boundary type - type of boundary for that zone = 1 - i0 boundary = 2 - idim boundary = 3 - j0 boundary = 4 - jdim boundary = 5 - k0 boundary

= 6 - kdim boundary

zone file - file name for zonal input deck

DUr	MY LINE
DUN	MY LINE
The next SET of lines is repeate	
DUN	
	OUP INFO ####################################
****** end of zona	al boundary info ****************
Same as zonal boundary line other side of the zonal bou	
	oundary line 4 ***************
DUN	MMY LINE
other side of the zonal bou	undary.
Same as zonal boundary line	
DUI	MMY LINE
mapping - mapping of state (List should be #	variables from other zone into this one var long)
<pre># var - # of state varibles</pre>	
****** zonal b	oundary line 2 ****************
	MMY LINE
end2 - ending value for dir	
start2 - starting value for	r dir2 variable
	f grid in zone that corresponds to other side of zonal boundary
end1 - ending value for dir	cl variable
start1 - starting value for	r dirl variable
	f grid in zone that corresponds to other side of zonal boundary

starting zone - first zone in this group

ending zone - last zone in this group

NOTE: zones must be ordered such that the zone numbers for each group are sequential.

imarch - space marching flag

- = 0 solve using global iterations
- = 1 space march, Stop calculation if tolerances on a plane are not met in nit iterations.
- =-1 space march, do NOT stop on an i plane if tolerances are not me. Proceed to next i plane and continue calculation.

nseq - number of levels of mesh sequencing performed for the group

NOTE: Every group must have nseq >= 1, if no sequencing is being performed, set nseq = 1

************** sequence info line 1 ************

----- DUMMY LINE ------

This sequence info line is repeated for each zone in the group (from starting zone to ending zone)

zone # - zone #'s in increasing order

ilevel - level of coarsening in i-direction

jlevel - level of coarsening in j-direction

klevel - level of coarsening in k-direction

NOTE: The sequencing is performed separately in each direction. A coarsening level of 1 corresponds to the finest mesh (or NO mesh sequencing). A level of 2 corresponds to every other grid line. A level of 3 corresponds to every third grid line, and so on. In order to coarsen a given direction to a certain level, the following constraint on the grid dimension must apply:

(dimension-1) must be exactly divisible by the coarsening level. For example: the remainder of (idim-1)/ilevel must be zero.

NOTE: Sequence Level #1 MUST correspond to the fine mesh, or ilevel = 1, jlevel = 1, klevel = 1

for all zones in this group

The terminology for this section is a bit confusing so here's an example :

sequence # 1 zone # ilevel jlevel klevel 1 1 1 1 sequence # 2 jlevel klevel zone # ilevel 1 3 1 sequence # 3 zone # ilevel jlevel klevel 1 3

In this example there are 3 sequencing levels (labeled #1, #2, & #3). Note that the higher the sequencing level, the coarser the mesh. The individual coarsening capability for each direction is apparent with the random choices shown. In going from sequence level 1 to 2 the mesh is coarsened 4, 3, and 0 times in the i, j, and k directions repectively. In going from sequence level 2 to 3 the mesh is coarsened 0, 0, and 2 times in the i, j, and k directions respectively since the coarsening level is relative and always refers back to the finest mesh.

************ end of sequence info *************
******************* end of group info *****************
######################################
DUMMY LINE
The next SET of lines is repeated for each block (NBLOCK times)
DUMMY LINE
DUMMY LINE
********************* block info line 1 *****************
igroup - group number for block
iseq - sequence level for block
<pre>nsweep - the number of different iteration types for this block. (note there must be at least one sweep for each zone in this block)</pre>
ncycle - number of cycles through each sweep
nwres - number of cycles performed in medium or high memory mode before the restart files are updated
rtolrg - normalized residual convergence criteria for this block

rtolag - absolute residual convergence criteria for this block
DUMMY LINE
Sweeping information is a subsection of the block info section. The following line is repeated NSWEEP times
*********** sweep info line 1 **************
sweep - sweep # in increasing order
zone - zone number corresponding to this sweep
<pre>isweep - time integration sweep direction = -/+ 1 - sweep in -/+ i-direction = -/+ 2 - sweep in -/+ j-direction = -/+ 3 - sweep in -/+ k-direction</pre>
NOTE: if space marching, isweep must be positive
<pre>nit - number of iterations to perform this sweep before continuing to the next sweep</pre>
istart - i/j/k dimension to start this sweep
iend - i/j/k dimension to end this sweep
*********** end of sweep info *************
********************* end of block info ******************

memmode - print memory mode flat

= 2 print out free stream quantities before each

line/set to standard ouput

^{= 0} low memory (Use this when printing multi-zone plot3d type files)

= 1 high memory mode, use this for most efficient
 line output calculation

******************* line/set specification line 1 ***********

iprint - flag for determining type of ouput file

= 1 line output prints to standard output, this output is suitable for display with 80 columns

- = 2 Tab delineated output prints each individual line to separate file each line prints variables in tab delineated format with one column per variable. Note, this is suitable for input into a line plotting package or spreadsheet type analysis package (i.e. Kaliedagraph on Mac)
- = 3 Integrated quantities use this option to print Cx, Cy, Cz, Cmx, Cmy, etc. to standard output (note, you must use this option in conjuction with either inode = 2,3, or 4)
- = 4 TECPLOT output
- = 5 PLOT3D ascii
 each line is treated as a separate grid in a
 plot3d ascii multi-grid format
 read/mg/form
 all plot3d ascii solutions written to file q.p3da
 a grid file is created by default labeled grid.p3da
- = 6 PLOT3D fortran binary each line is treated as a separate grid in a plot3d unformatted multi-grid format read/mg/unf all plot3d unformatted solutions written to q.p3du a grid file is created by default labeled grid.p3du (Note a conversion from gasp precision to machine single precision is performed i.e. on workstation real*8 are converted to real*4)
- = 7 PLOT3D c binary each line is treated as a separate grid in a plot3d binary multi-grid format read/mg/bin all plot3d binary solutions written to file q.p3db a grid file is created by default labeled grid.p3db (Note a conversion from gasp precision to machine single precision is performed i.e. on workstation real*8 are converted to real*4)

```
each line is treated as a separate grid in a
                plot3d binary multi-grid format
                for use on ieee workstations
                read/mg/bin
                 all plot3d binary solutions written to file q.p3dbi
                 a grid file is created by default labeled grid.p3dbi
                 (this option converts cray real*8 to ieee real*4)
                 NOTE: this is the most efficient way to use
                      plot3d or fast on a workstation from solution
                      created on a cray
     iout
             - flag for dimensionalizing output
             = 0 dimensional output (English units)
            = 1 dimensional output (SI units)
            = 2 non-dimensionalized by free stream
            = 3 non-dimensionalized by reference quantities
            NOTE: iout = 0, and iout = 1 are independent from the
                   iunits flag in the main gasp input deck
                   thus if you did the original calculation in SI
                   you can still view your solution in English units
    inode
            - flag for determining location of output
            = 0 output grid & q's at cell centers
            = 1 output grid & q's at grid nodes
            = 2 output quantities on i faces
             = 3 output quantities on j faces
            = 4 output quantities on k faces
            NOTE: inode = 2,3,4 currently MUST ONLY be used with
                  ivar = 601,602,603,611,612,613,621,622,623
                         701,702,703,711,712,713,721,722,723
    zone
            - zone number of output for that line
    seq -
              sequence number for output for that particular zone
   -----DUMMY LINE ------
************* line/set specification line 2 ***************
    this input line specifies the range of output for the specific
    line.
    valid ranges
      inode = 0 (cell centered)
          [0:idim][0:jdim][0:kdim]
         note 0 and dim are at the boundaries
      inode = 1 (nodal output)
          [1:idim] [1:jdim] [1:kdim]
         note 1 and dim are at the boundaries
      inode = 2 (i faces)
          [1:idim] [1:jdim-1] [1:kdim-1]
      inode = 3 (j faces)
          [1:idim-1][1:jdim][1:kdim-1]
      inode = 4 (k faces)
          [1:idim-1][1:jdim-1][1:kdim]
    i1
            - starting i indices for output
    i2
            - ending i indices for output
    iinc
            - i increment for output
    j1
            - starting j indices for output
```

C

= 8 PLOT3D iris c binary (only supported on cray)

- ending j indices for output **†**2 jinc - j increment for output k1 - starting k indices for output k2 - ending k indices for output kinc - k increment for output Note: Regardless of the mesh sequencing level, dimensions given to this line are with respect finest mesh -----DUMMY LINE --------*********** line/set specification line 3 ******************* number of variables to be printed list of variables to be printed (numbers correspond to plot3d function numbers where applicable) supported functions x coordinate y coordinate 3 z coordinate 50 laminar viscosity 51 laminar thermal conductivity 60 mixture gamma 70 Turbulent Kinetic Energy (K) per unit mass 71 TKE dissipation rate (Epsilon) per unit mass 72 Turbulent Kinetic Energy (Rho K) per unit volume 73 TKE dissipation rate (Rho Epsilon) per unit volume 100 Mixture Density 110 Pressure 114 Pressure Coefficient 120 Temperature 132 Stagnation Enthalpy per unit mass 142 Stagnation Energy per unit mass 150 U Velocity 151 V Velocity 152 W Velocity 154 Mach Number 155 Speed of Sound 160 X-Momentum 161 Y-Momentum 162 **Z-Momentum** 163 Stagnation Energy per unit volume 501 Skin Friction Coefficient on I faces 502 Skin Friction Coefficient on J faces 503 Skin Friction Coefficient on K faces Note 501,502,503 are defined as the coefficient due to

the magnitude viscous forces tangent

to the I,J, or K faces

511 512 513	Heat Transfer Coefficient on I faces Heat Transfer Coefficient on J faces Heat Transfer Coefficient on K faces
601 602 603	total force on a face in the x direction total force on a face in the y direction total force on a face in the z direction
611 612 613	Pressure force on a face in the x direction Pressure force on a face in the y direction Pressure force on a face in the z direction
621 622 623	Viscous force on a face in the x direction Viscous force on a face in the y direction Viscous force on a face in the z direction
	Note: 601,602,603,611,612,613 are only valid

for inode = 2,3,or 4

******************* end of print input ******************

Zonal input deck, (one for each zone)

The input deck for each zone is organized into 5 basic sections

- 1) Problem Specification
 - a) grid size, # species, etc
 - b) free stream quantities
 - c) boundary condition information
- 2) Time Integration
 - a) time integration technique
 - b) cfl number
 - c) reuse of LU decomp parameters
 - d) marching support parameters
- 3) Inviscid Fluxes
 - a) type of flux & Jacobian used
 - b) variable interpolation & limiters
- 4) Viscous Fluxes
 - a) flux & Jacobian control
 - b) transport property model parameters
 - c) Prandtl & Schmidt numbers
 - d) turbulence parameters
- 5) Chemistry & Thermodynamics
 - a) chemistry & thermodynamic model
 - b) frozen, equil., & finite rate source term & Jacobian control parameters

********	#### PROBLE	M SPECIFICA	TION ######	############	####
******	problem spe	ecification	line 1 ****	*****	****
title card					
	DU	MMY LINE			

idim - grid size in i direction

jdim - grid size in j direction

kdim - grid size in k direction

nspec - number of chemical species

nnev - number of nonequilibrium energy contributions

NOTE: grid dimension correspond to finest mesh in mesh sequencing coarser grid dimensions are determined from mesh sequencing

	DUMMY LINE
******	****** problem specification line 3 ***************
icond	 input initialization flag 1 velocity components and temperature are input 2 Mach number components and temperature are input 3 velocity components and pressure are input 4 Mach number components and pressure are input
U,V,W	 free stream velocity components (units of velocity must correspond to selection of iunits flag in the main input deck)
Mx,My,Mz	- free stream Mach number components
T,p	 free stream temperature/pressure (units of pressure or temperature must correspond to selection of iunits flag in the main input deck)
xkiv	<pre>- free stream value of turbulent intensity Kinf = (xkiv*Vinf)^2 (units are important)</pre>
tkelre	<pre>f - reference length for calculation of free stream epsilon or turbulent reynolds number. > 0 reference length input < 0 turbulent reynolds number input (L=-tkelref/xkiv/Re) eps = K^(3/2)/L, also eddy viscosity = rho*sqrt(K)*L. (units are important)</pre>
	DUMMY LINE
******	****** problem specification line 4 ***********************************
	DUMMY LINE
*****	******* problem specification line 5 **************
	 implicit boundary condition flag 0 - explicit boundary conditions 1 - implicit boundary conditions
- - - -	 initialization flag for boundary conditions this is only used if the corresponding boundary condition has type 2 values where q's are read in from a file. It allows the domain to be initialized with profiles that are read in this way. 0 - do nothing 1 - initialize q's zone with i0 boundary values 2 - initialize q's zone with idim boundary values 3 - initialize q's zone with j0 boundary values 4 - initialize q's zone with jdim boundary values 5 - initialize q's zone with k0 boundary values 6 - initialize q's zone with kdim boundary values

i0bc - i0 boundary condition flag idimbc - idim boundary condition flag

j0bc - j0 boundary condition flag

jdimbc - jdim boundary condition flag

k0bc - k0 boundary condition flag

kdimbc - kdim boundary condition flag

boundary conditions :

- do a point by point description of boundary
- fixed at the freestream conditions
- fixed at the values read from a file
- first order extrapolation
- second order extrapolation
- characteristic b.c.s (subsonic inflow/outflow)
- subsonic inflow total pressure and temperature fixed subsonic outflow - back pressure specified
- = 8 tangency
- = 9 no-slip, adiabatic wall
- = 10 no-slip, T fixed at wall
- = 11 x-axis symmetry (j or k) - singular axis
- y-axis symmetry (j or k) singular axis z-axis symmetry (j or k) singular axis = 12
- **=** 13
- = 14 xy-plane axisymmetric singular axis
- = 15 singular axis yz-plane axisymmetric
- = 16 xz-plane axisymmetric singular axis
- = 17 reflection x-axis
- = 18 reflection y-axis
- = 19 reflection z-axis
- zonal boundary (fills q with adjacent zone values)
- axisymmetric wall (negative pi/80 angle)
- = 22 axisymmetric wall (positive pi/80 angle)

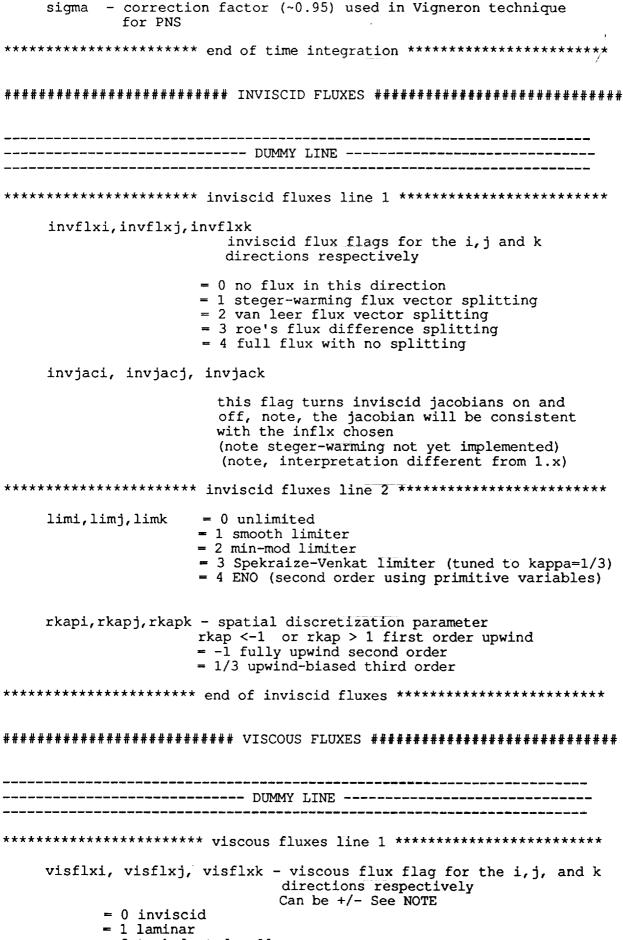
positive boundary type enforces full flux at boundary negative boundary type splits the flux at boundary

- NOTES: 1) Types 8,9,10 are enforced on the cell faces, the others are enforced at the cell centers.
 - Types 11, 12, 13 are typically used for grids that vary between 0 and 180 degrees in a cross-flow plane.
 - 3) Types 14, 15, 16 are typically used for grids that are a pie-slice (axisymmetric) in the crossflow plane.
 - 4) Types 17, 18, 19 should always be negative
 - 5) Types 21, 22, should always be positive
 - 6) Types 5 and 6 use perfect gas relations!

pback - back pressure for boundary condition 6

DUMMY LINE
******** problem specification line 6 ***************
twall - wall temperature for boundary condition 10

```
- total temperature for boundary condition 6
        - total pressure for boundary condition 6
    ptot
    (UNITS ARE IMPORTANT)
  ------
************* problem specification line 7 ****************
    Name of file containing boundary condition type for each point on
    all boundaries with type '0' above. and name of qfile for bc
    type 2's. these filenames MUST be enclosed in single quotes
************* end of problem specification ****************
-----DUMMY LINE ------
***************** time integration line 1 ******************
    impl - time integration method flag
        = 0 explicit Runge-Kutta time integration
        = 1 LU decomposition in a on a line (only for 2-d problems)
= 2 2-Factor AF in a plane
= 3 3-Factor AF
    mstg - number of stages for Runge-Kutta
    dt
         time step
        < 0 local time steps, cfl=abs(dt)</pre>
        > 0 constant time step = dt
    initdtl - flag for cfl calculation
        = 0 - use freestream q
        = 1 - use local values of q
  ----- DUMMY LINE -----
************** time integration line 2 ****************
    irelu - reuse of LU decomposition flag
        = 0 - compute LU decomposition every time step
        = 1 - reuse LU decomposition based on tolreu & nremax
        = -NUM - begin reusing LU after NUM iterations
    nremax - maximum number of reuses before computing new LU decomp
    tolreu - tolerance of residual at which to begin reusing LU decomp
    initp - only used if imarch=1
          = 0 fill new plane with free stream values
          = 1 fill new plane with converged solution of
           previous plane
```



^{= 2} turbulent 0 wall

^{= 3} turbulent dim wall

= 4 turbulent both j walls

NOTE: ivisci, iviscj, and ivisck can be chosen in various combinations of + or - values. '-' values give thin-layer contributions, '+' values in combination with other '+' values add to the thin-layer terms the cross-derivative contributions.

Example, ivisci=-1, iviscj=1, ivisck=1 includes crossin derivatives the j-k plane. Thus, ivisci, j, k=+1 gives Complete Navier-Stokes terms and would be a laminar calculation. The choice ivisci=+1, iviscj=+4, ivisck=+4 would also be a Complete Navier-Stokes calculation and would be a turbulent simulation in which the composite eddy viscosity is computed by combining distributions calculated from the j0, k0, jdim, and kdim surfaces.

visjaci, visjacj, visjack - viscous flux jacobian for the i,j, and k directions respectively

- = 0 no jacobian in that direction

= 1 thin layer jacobian in that direction ------DUMMY LINE -------modlmu - laminar viscosity model = 1 Blottner curve fit for species laminar viscosity= 2 Sutherland formula for species laminar viscosity = 3 Keys Equation (perfect gas model only (0) valid for air! = 4 Helium tunnel equation w/Blottner curve fits (helium-n2-o2 model only (24)) = 5 Helium tunnel equation w/Sutherland curve fits (helium-n2-o2 model only (24)) modlk - thermal conductivity model = 1 Euken relation for species thermal conductivity = 2 Sutherland formula for species thermal conductivity = 3 mixture thermal conductivity evaluated using a constant Prandtl number modld - diffusion model = 1 simple binary diffusion prl - Prandtl number (only used if modlk=3) prt - turbulent Prandtl number scl - laminar Schmidt number

----- DUMMY LINE -----

ikeps - flag for two equation model used

- turbulent Schmidt number

- = 0 Baldwin-Lomax algebraic model
- = 1 High Reynolds # model
- = 2 Lam-Bremhorst model
- = 3 Chien model

sct

```
= 0 - no Jacobian
           = 1 - compute source term Jacobians
    NOTE: If you want to run a completely laminar calculation,
          ikeps must be 0.
            - flag for imposing minimum value for K & e
    kemin
             = 0 - do nothing
             = 1 - impose minimum value based on small percentage
                   of free stream values of K & epsilon
       NOTE: This adds stability, but the results may then be
             dependent on values of xkiv & tkelref chosen. It
             is suggested that this be used in the early stages of
             iteration or with only a small value for xkiv.
    kefill - flag to initialize TKE with eddy viscosity &
              mixing length from Baldwin-Lomax solution
           = 0 do nothing
           = 1 init with B L solution
     *** NOTE: Turn this off after initialization!!!!! ***
****************** end of viscous fluxes *****************
----- DUMMY LINE -----
******* chemistry & thermodynamics line 1 ***********
    itherm - thermodynamic model
           = 1 - equilibrium statistical mechanics model for species
           internal energy ( translation + rotation + vibration )
= 2 - curve fit for Cv (Gordon and McBride)
           = 3 - simplified vibrational relaxation model for species
                 internal energy
           = 4 - translation + rotation only (mixture of perfect gas)
           = 5 - liu equilibrium air curve fits
           = 6 - tgas equilibrium air curve fits
    chemfile - chemistry model file name in Inits/models.sum file
             'Perfect Gas' - Perfect Gas model
             'Kang & Dunn' - Kang and Dunn Air model
             'Park 1' - first Park Air model
             'Park 2' - second Park Air model
             'Park 3' - third Park Air model
              'Evans & Schexnayder 1' - first Evans & Schexnayder
                                     Hydrogen-Air model
              'Evans & Schexnayder 2' - second Evans & Schexnayder
                                      Hydrogen-Air model
              'Drummond 1' - first Drummond Hydrogen-Air model
              'Drummond 2' - second Drummond Hydrogen-Air model
              'NASP 1' - first NASP Hydrogen-Air model
              'NASP 2' - second NASP Hydrogen-Air model
              'NASP 3' - third NASP Hydrogen-Air model
             'NASP 4' - fourth NASP Hydrogen-Air model
             'Glass' - Glass model
             'Igra' - Igra model
              'Argon-Freon Plasma' - Argon-Freon Plasma model
```

ikejac - two equation Jacobian flag

- 'Equilibrium Air' Equilibrium Air model
- = 'Evans & Schexnayder 3' second Evans & Schexnayder hydrogen air model (Same reactions as 1.x)

ieq -

- = 1 frozen flow
- = 2 chemical equilibrium flow
- = 3 chemically reacting flow

(Warning - ieq flag definitions are different from 1.x)

ichjac - chemical Jacobian flag

- = 0 no Jacobian
- = 1 compute chemical Jacobian (no temperature derivatives)
 = 2 compute chemical Jacobian (full linearization)

******* end of chemistry & thermodynamics **********